WHAT IS CLAIMED IS:

1.   A method of drug discovery and development comprising using one or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs to identify compounds that have desired activity at two or more molecular targets that are associated with a disease state for which the drug discovery and development are directed.

2.   The method of claim 1, wherein the drug discovery and development are directed to identifying additional applications and uses of known compounds.

3.   The method of claim 1, wherein the drug discovery and development are directed to identifying multiple targets relevant to the treatment of a specific disease state.

4.   The method of claim 1, wherein the drug discovery and development are directed to *in silico* identification of compounds that display patterns of activity at two or more molecular targets that are associated with a disease state.

5.   A method of drug discovery and development comprising using one or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs to identify compounds that (a) have desired activity at one or more molecular targets that are associated with a disease state for which the drug discovery and development are directed and (b) do not have activity or have substantially reduced activity that is undesired at one or more molecular targets that are associated with possible side effects; toxicity; adverse absorption, distribution, metabolism, or elimination (ADME) properties; or other properties not intended to be manifested by compounds being developed to treat the disease state associated with the drug discovery.

6.   The method of claim 5, wherein the drug discovery and development are directed to identifying additional applications and uses of known compounds.

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7. The method of claim 5, wherein the drug discovery and development are directed to identifying multiple targets relevant to the treatment of a specific disease state.

8. The method of claim 5, wherein the drug discovery and development efforts are directed to *in silico* identification of compounds that display patterns of activity and inactivity at two or more molecular targets that are associated with a disease state.

9. A method of drug discovery comprising:

selecting two or more molecular targets related to a cause or mechanism of a disease, disease process or medical condition;

accessing a dataset comprising results of tests of interactions between each of the selected targets and a multiplicity of chemical compounds, wherein the chemical compounds may be described by descriptors related to features of the compounds;

establishing criteria for selecting, and then selecting a set of active compounds comprising those chemical compounds that demonstrate activity in the tests of interactions between the targets and compounds, for each of the selected molecular targets;

assembling sets of descriptors identified with those compounds comprising the set of selected active compounds, for each of the selected molecular targets;

identifying from the sets of assembled descriptors for each selected molecular target those descriptors that are found in common for each combination of two or more of the selected molecular targets; and

identifying, using the identified in common descriptors, chemical compounds useful for drug discovery purposes related to a disease, disease process, or medical conditions to which the selected molecular targets are related.

10. The method of claim 9, further comprising:

using the identified in common descriptors to access a set of chemical compounds suitable for drug discovery, such compounds being encoded by descriptors that include a form of descriptors used for the method of claim 9;

searching the set of compounds suitable for drug discovery for the presence of the identified in common descriptors and selecting those chemical compounds from the set of

compounds suitable for drug discovery that have the features represented by the identified in common descriptors; and

obtaining such selected chemical compounds for use in drug discovery screening processes directed toward a disease, disease process, or medical condition or for other drug discovery purposes.

11.   The method of claim 9, wherein the identified in common descriptors are used for design or synthesis of new compounds.

12.   The method of claim 11, wherein the design or synthesis of new compounds is directed toward drug discovery related to a disease, disease process, or medical conditions to which the selected molecular targets are related.

13.   The method of claim 9, wherein the molecular targets are receptors, enzymes, transporters, uptake sites, ion channels, proteins, nucleic acids, carbohydrates, or polysaccharides.

14.   The method of claim 9, wherein the disease, disease process, or medical condition is cocaine addiction, attention deficit hypersensitivity disorder, Parkinson's disease, anxiety, depression, obesity, or barbiturate abuse.

15.   The method of claim 9, wherein the dataset of interactions is from a receptor selectivity mapping database.

16.   The method of claim 9, wherein the interactions are measured by binding, interaction between a compound known to interact with a target and the target, functional activation, functional enhancement, functional inhibition, or lack of function effect with respect to a molecular target.

17.   The method of claim 9, wherein descriptor types are 2-dimensional distance geometries, 3-dimensional distance geometries, sub-structural components, molecular volumes,

charge distributions, charge distributions, atom types, or descriptors derived by means of physicochemical depiction of a small molecule.

18.   The method of claim 9, wherein the selection criteria are dependent on desired or undesired properties of the selected molecular targets.

19.   A method for identifying or designing a chemical compound that has desired characteristics and interacts with one or more selected molecular targets, comprising:

selecting one or more positive molecular targets for which a positive interaction with a chemical compound is desired and one or more negative molecular targets for which a lack of significant interaction with the same chemical compound is desired;

accessing a dataset comprising results of tests of interactions between each of the selected positive and negative targets and a multiplicity of chemical compounds, wherein the chemical compounds may be described by descriptors related to features of the compounds;

establishing a threshold or other criteria for selecting, and then selecting a set of active compounds comprising those chemical compounds that demonstrate a desired positive interaction or activity in the tests of interactions between the targets and compounds, for each of the selected positive targets;

establishing a threshold or other criteria for selecting, and then selecting a second set of active compounds comprising those chemical compounds that demonstrate an undesired positive interaction or activity in the tests of interactions between the targets and compounds, for each of the selected negative targets;

assembling sets of positive descriptors that are identified with the compounds comprising the set of selected active compounds for the positive targets;

assembling sets of negative descriptors that are identified with the compounds comprising the second set of selected active compounds for the negative targets; and

using the positive descriptors and negative descriptors to identify or design chemical compounds having characteristics indicative of the positive descriptors but lacking characteristics indicative of the negative descriptors.

20. The method of claim 19, further comprising wherein the positive descriptors and negative descriptors are further used for identifying a chemical compound that has desired characteristics by:

using the positive descriptors and negative descriptors to identify a chemical compound having desired characteristics by accessing a set of chemical compounds potentially suitable for an intended purpose or use, the set of potentially suitable chemical compounds being encoded by descriptors that include a form of descriptors used for the method of Claim 12;

searching the set of potentially suitable chemical compounds for the presence of the positive descriptors and selecting a subset of chemical compounds with characteristics indicated by the positive descriptors;

searching the subset of chemical compounds for the presence of the negative descriptors and eliminating chemical compounds from the subset of chemical compounds that have characteristics indicated by the negative descriptors; and

obtaining and further using or testing the eliminated chemical compounds for the intended purpose.

21. The method of claim 20, further comprising obtaining and further using or testing compounds remaining in the subset after having eliminated the chemical compounds that have characteristics indicated by the negative descriptors.

22. The method of claim 20, wherein the set of chemical compounds comprises synthetic chemicals, small organic molecules, natural products, virtual compounds, a virtual library, or drug-like compounds.

23. The method of claim 19, further comprising:

using the positive descriptors and negative descriptors to identify a chemical compound having desired characteristics by accessing a set of chemical compounds potentially suitable for an intended purpose or use, the set of potentially suitable chemical compounds being encoded by descriptors that include a form of descriptors used for the method of claim 12;

searching the set of potentially suitable chemical compounds for the presence of the negative descriptors and eliminating chemical compounds that have characteristics indicated by the negative descriptors;

searching the set of potentially suitable chemical compounds corresponding to remaining compounds for the presence of the positive descriptors and selecting chemical compounds from the remaining compound set that have characteristics indicated by the positive descriptors; and

obtaining and further using or testing the selected remaining compounds for the intended purpose.

24. The method of claim 19, wherein the positive and negative descriptors are used for design of chemical compounds having characteristics indicated by the positive and negative descriptors.

25. The method of claim 24, wherein the designed compounds are synthesized and further used or tested for the intended purpose.

26. The method of claim 19, wherein the method is used for drug discovery or development.

27. The method of claim 19, wherein the positive targets are related to the cause or mechanism of a disease, disease process or medical condition.

28. The method of claim 19, wherein the positive targets are receptors, enzymes, transporters, uptake sites, ion channels, proteins, nucleic acids, carbohydrates, macromolecules, or polysaccharides.

29. The method of claim 19, wherein the negative targets are related to the cause or mechanism of drug side effects, drug adverse effects, toxicity effects, toxicological effects, undesired pharmacokinetic properties, or undesirable effects of administration of pharmaceuticals.

30.   The method of claim 19, wherein the negative targets are receptors, enzymes, transporters, uptake sites, ion channels, proteins, nucleic acids, carbohydrates, macromolecules, or polysaccharides.

31.   The method of claim 19, wherein the dataset comprises results of tests of interactions between each of the selected targets and a multiplicity of chemical compounds in a full-rank dataset.

32.   The method of claim 19, wherein the dataset comprises results of tests of interactions between each of the selected targets and a multiplicity of chemical compounds that contains positive and negative interaction test results.

33.   The method of claim 19, wherein each compound in the dataset has been tested against each target in the dataset, results of each such test being recorded in a database including the dataset.

34.   The method of claim 19, wherein the tests of interactions measures an effect that each compound has on an interaction of a compound known to interact with a specific molecular target from the selected positive and negative targets and the specific molecular target.

35.   The method of claim 34, wherein the tests of interaction comprise a competitive binding assay.

36.   The method of claim 19, wherein the tests of interactions comprise a binding assay.

37.   The method of claim 19, wherein the tests of interactions comprise a functional assay.

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